Pattern formation during Rayleigh-Bénard convection in non-Boussinesq fluids

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Abstract

Motivated by recent experimental studies of Bodenschatz et al. [E. Bodenschatz, J.R. de Bruyn, G. Ahlers and D.S. Cannell, Phys. Rev. Lett. **67**, 3078 (1991)], we present a numerical study of a generalized two dimensional Swift-Hohenberg equation to model pattern formation in Rayleigh-Bénard convection in a non-Boussinesq fluid. It is shown that many of the features observed in these experiments can be reproduced by this generalized model that explicitly includes non-Boussinesq and mean flow effects. The spontaneous formation of hexagons, rolls, and a rotating spiral pattern is studied, as well as the transitions and competition among them. Mean flow, non-Boussinesq effects, the geometric shape of the lateral wall, and sidewall forcing are all shown to be crucial in the formation of the rotating spirals. We also study nucleation and growth of hexagonal patterns and find that the front velocity in this two dimensional model is consistent with the prediction of marginal stability theory for one dimensional fronts.

1 Introduction

One of the most striking examples of spatio-temporal self-organized phenomena in nonequilibrium systems is the rotating spiral states observed in chemical and biological systems [1]. It is remarkable that such time dependent but macroscopically coherent states can be sustained in systems that are not in equilibrium. The Belousov-Zhabotinsky reaction [2], for example, has received considerable attention as an example of a chemical wave propagation. Spiral patterns in this system result from the coupling of reaction and transport processes.

Recently, similar rotating spiral patterns have been observed in Rayleigh-Bénard convection in non-Boussinesq fluids in large aspect ratio systems [3]. According to the classical work of Busse [4], the first bifurcation from the conducting state is to a convective state of hexagonal symmetry. Convective cells form a stationary honeycomb structure. Further away from threshold, the system undergoes a new bifurcation to a state comprising parallel convective rolls (roll patterns are the only patterns predicted and observed within the Boussinesq approximation. The existence of of a stationary pattern of hexagonal symmetry is a direct consequence of deviations from the Boussinesq approximation). The predicted bifurcation from hexagons to rolls is direct, so that the fluid is expected to evolve to a stationary patterns of rolls. Recently, however, experiments on convection in CO_2 gas by Bodenschatz et al. [3] show that the system has a tendency to spontaneously form rotating spirals. These rotating states are long lived, and do not decay to the expected pattern of concentric rings (in a circular geometry). Furthermore, depending on the value of the Rayleigh number, spirals with a different number of arms have been observed.

Rayleigh-Bénard convection in monocomponent fluids is governed by the full three dimensional fluid equations. Because of the difficulty in solving the three dimensional initial value problem posed by the fluid equations, we and others have focused on the study of simpler two dimensional model equations. An example of such models is

the so-called "Swift-Hohenberg" (SH) equation, which is asymptotically equivalent to the long distance and long time behavior of the fluid equations near onset of convection and in the Boussinesq approximation [5, 6, 7]. A great deal of theoretical and numerical work on this latter model has been done by Cross [8], and by Greenside et al. [9], but much remains to be done in non-Boussinesq systems, even within the framework of a SH-type equation.

We study in this paper a generalized SH equation that includes both a quadratic nonlinearity and coupling to mean flow effects. The values of the parameters that enter the equation have been chosen to be in the range appropriate for the experiments of Bodenschatz et al. We find that stable rotating spirals are spontaneously formed during the hexagon to roll transition, in agreement with the experimental observations. The quadratic nonlinearity in the equation is responsible for the rotational symmetry breaking and leads, by itself, to stationary spiral patterns. When coupling to mean flow in included, and therefore when the model equation is not potential, the same transition leads to rotating spirals instead. However, spirals are not obtained if one sets the quadratic term equal to zero but keeps the mean flow term. Sidewall forcing also seems to be essential in obtaining this pattern. Otherwise, rolls that are locally perpendicular to the sidewall appear and no uniformly rotating state is observed. Finally, once the spiral state is formed, it is unstable to the removal of the quadratic nonlinearity in the equation. The spiral state quickly decays to a set of concentric rings.

We note that Bestehorn et al. [10] have reported a numerical study of this very same model to study the rotation of a spiral pattern, but their study is limited to the special case in which the initial configuration is a spiral. The fundamental question addressed in our work is, in contrast, how the spiral pattern is spontaneously formed during the hexagon to roll transition.

In Section II, we give a brief description of the theoretical model used to describe

pattern formation in non-Boussinesq systems, and in Section III we provide a detailed description of the numerical method for solving the model equation. In Section IV, we present various numerical results, show in detail the hexagonal and spiral patterns and compare our results with the experiments of Bodenschatz et al. In Section V, we present a brief summary.

2 A two dimensional model equation for convection in non-Boussinesq fluids

A great deal of our current understanding of the spatial and temporal properties of convective patterns near onset has been obtained by using model equations such as the Swift-Hohenberg (SH) equation, which in dimensionless variables takes the following simple form [5, 11],

$$\frac{\partial\psi(\vec{r},t)}{\partial t} = \left[\epsilon - \left(\nabla^2 + 1\right)^2\right]\psi - \psi^3, \tag{1}$$

where $\vec{r}$ is a two dimensional vector lying in the (x, y) plane (the convective cell is parallel to this plane), and ϵ is the control parameter. This equation describes the evolution of a single scalar field ψ which is commensurate with the convective rolls. When $\epsilon > 0$, this equation has roll-like solutions with a wavenumber $q = 1$. This equation can also be written in potential form,

$$\frac{\partial\psi}{\partial t} = -\frac{\delta\mathcal{L}}{\delta\psi}, \tag{2}$$

where $\mathcal{L}$ is a Lyapunov functional. The dynamical evolution of ψ is naturally interpreted in terms of the minimization of this functional. Therefore a potential system cannot display either the oscillatory or aperiodic time dependence observed in the experiments. Although potential systems are quite important for the understanding of the features of the emerging patterns, an interesting question one may ask is which flow component is necessary to describe the observed non-potential behavior. One

such component is the so-called large scale mean flow, which was first proposed by Siggia and Zippelius [12].

Large scale mean flows are composed of one particular spatial harmonic of the basic roll pattern. In the case of free-free boundary conditions, this harmonic corresponds to a flow that is independent of z, the coordinate normal to the convective cell plates. This flow is not damped in the (unrealistic) case of free-free boundary conditions, and is only slightly damped in the more realistic case of rigid-rigid boundary conditions. Since the nonlinear term in the fluid equations that gives rise to large scale mean flow is not $\vec{v} \cdot \nabla\theta$, but $\vec{v} \cdot \nabla\vec{v}$, the magnitude of the large scale flow is inversely proportional to the Prandtl number. Moreover, for a perfect straight roll pattern, no large scale mean flow is generated; it appears only when rolls are bent or modulated. In that case, the characteristic length scale of these flows is large compared with the roll wavelength. For example, the large scale mean flow contribution to the SH equation [12, 13] has been shown to play a key role in the onset of weak turbulence in Boussinesq systems [14].

We next describe a two dimensional model of convection in a non-Boussinesq fluid. We use the two dimensional generalized Swift-Hohenberg (GSH) equation [5, 9, 13], given by Eqs. (3) and (4) below, which we solve by numerical integration. Our model in dimensionless units is defined by,

$$\frac{\partial\psi(\vec{r},t)}{\partial t} + g_m\vec{U}\cdot\nabla\psi = \left[\epsilon - \left(\nabla^2+1\right)^2\right]\psi - g_2\psi^2 - \psi^3 + f(\vec{r}), \tag{3}$$

$$\left[\frac{\partial}{\partial t} - Pr(\nabla^2 - c^2)\right]\nabla^2\xi = \left[\nabla(\nabla^2\psi\times\nabla\psi)\right]\cdot\hat{e}_z, \tag{4}$$

where,

$$\vec{U} = (\partial_y\xi)\hat{e}_x - (\partial_x\xi)\hat{e}_y, \tag{5}$$

with boundary conditions,

$$\xi|_B = \hat{n}\cdot\nabla\xi|_B = \psi|_B = \hat{n}\cdot\nabla\psi|_B = 0, \tag{6}$$

where $\hat{n}$ is the unit normal to the boundary of the domain of integration, B. If the coupling to large scale flow is dropped ($g_m = 0$), Eq. (3) is potential. Also this equation reduces to the dimensionless SH equation (Eq. (1)) when the coupling coefficients $g_2 = g_m = 0$. As is the case in Eq. (3), the scalar field $\psi(\vec{r}, t)$ is proportional to a linear combination of the fluid temperature modulation and vertical velocity fields at a point $\vec{r}$ in the midplane of the fluid layer, parallel to the upper and lower walls of the convective cell. $\xi(\vec{r}, t)$ is the vertical vorticity potential [12, 13, 14]. The quantity ϵ is the control parameter. Pr is the Prandtl number of the fluid, $\hat{e}_x$ and $\hat{e}_y$ are two unit vectors parallel to the x and y direction respectively, and c^2 is an unknown constant. A phenomenological forcing field f has been included in Eq. (3) to simulate lateral sidewall forcing produced by horizontal temperature gradients present in the experiments. As in earlier studies [15, 16], we have varied the strength and spatial extent of f in order to match the experimental observations. In order to estimate the values of the various dimensionless parameters that enter the GSH equation in terms of experimentally measurable quantities, we have derived a three mode amplitude equation (see the Appendix for details). From the experiments described in reference [3], we estimate that $g_2 = 0.35$, $g_m = 50$, $c^2 = 10$ and $Pr = 1$. The value of ϵ used in the numerical calculation is related to the experimental value ϵ_{expt} by $\epsilon_{expt} = 0.3594\epsilon$.

3 Numerical method

The numerical method for solving the GSH equation (Eqs. (3) - (6)) is based on the elegant work by Greenside et al. [9], and Bjørstad et al. [17]. We sketch below their numerical scheme. The key step is to recognize that the GSH equation can be solved by the repeated solution of the *linear* constant coefficient biharmonic equation for a function u,

$$(\nabla^2\nabla^2 + a\nabla^2 + b)u = f_1, \tag{7}$$

with boundary conditions,

$$u|_R = f_2, \quad \hat{n} \cdot \nabla u|_R = f_3, \tag{8}$$

on a circular domain R. The constants a and b are real numbers, $\hat{n} \cdot \nabla$ denotes the normal derivative taken at the boundary of the domain, and f_1 , f_2 and f_3 are given functions. For the case of rigid boundaries, we have $f_2 = f_3 = 0$.

Consider an *implicit* backward Euler discretization scheme in time, to yield the following finite difference set of equations for Eqs. (3)-(6),

$$\begin{aligned} &\frac{\psi(\tau+\Delta\tau) - \psi(\tau)}{\Delta\tau} + g_m \vec{U}(\tau+\Delta\tau) \cdot \nabla\psi(\tau+\Delta\tau) = \\ &\qquad L\psi(\tau+\Delta\tau) - g_2\psi^2(\tau+\Delta\tau) - \psi^3(\tau+\Delta\tau), \end{aligned} \tag{9}$$

$$\begin{aligned} &\frac{\nabla^2\left[\xi(\tau+\Delta\tau) - \xi(\tau)\right]}{\Delta\tau} + Pr\nabla^2\left[c^2 - \nabla^2\right]\xi(\tau+\Delta\tau) = \\ &\qquad -\left[\nabla\psi(\tau+\Delta\tau) \times \nabla(\nabla^2\psi(\tau+\Delta\tau)\right] \cdot \hat{e}_z, \end{aligned} \tag{10}$$

where $\psi(\tau)$ and $\xi(\tau)$ are the known solutions of Eqs. (3)-(4) at time τ, $\Delta\tau$ is the time step, $L = \epsilon - (1+\nabla^2)^2$ is a linear biharmonic operator, and $\psi(\tau+\Delta\tau)$ and $\xi(\tau+\Delta\tau)$ are the unknown implicit solutions at the next time step $(\tau+\Delta\tau)$ (we have temporarily suppressed the spatial arguments). We solve Eqs. (9) and (10) by using a multi-iteration Gauss-Seidel scheme. We first assume that $\psi(\tau+\Delta\tau)$ and $\xi(\tau+\Delta\tau)$ are obtained by successive approximations of the form,

$$\psi(\tau+\Delta\tau) \simeq \psi_{k+1} = \psi_k + \delta_k, \quad \text{with} \psi_0 = \psi(\tau), \tag{11}$$

$$\xi(\tau+\Delta\tau) \simeq \xi_{k+1} = \xi_k + \theta_k, \quad \text{with} \xi_0 = \xi(\tau), \tag{12}$$

where ψ_k and ξ_k are the approximations at the $k-th$ iteration. The equation satisfied by the so-called outer correction fields, δ_k and θ_k, can be obtained (assuming $\| \delta_k \| \ll \| \psi_k \|$ and $\| \theta_k \| \ll \| \xi_k \|$ in the maximum norm). By substituting Eqs. (11) and (12) into Eqs. (9) and (10), and linearizing them with respect to δ_k and θ_k, we then obtain the standard Gauss-Seidel iteration scheme for the unknown corrections δ_k and θ_k,

$$\left[L - 3\psi_k^2 - 2g_2\psi_k - \frac{1}{\Delta\tau}\right]\delta_k = \frac{\psi_k - \psi_0(\tau)}{\Delta\tau} + g_m\vec{U}_k \cdot \nabla\psi_k - (L\psi_k - \psi_k^3 - g_2\psi_k^2), \tag{13}$$

$$\nabla^2\left[\nabla^2 - h^2\right]\theta_k = -\frac{1}{Pr\Delta\tau}\nabla^2\xi_0 - \nabla^2\left[\nabla^2 - h^2\right]\xi_k$$
$$+\frac{1}{Pr}\left[\nabla\psi_{k+1}\times\nabla(\nabla^2\psi_{k+1})\right]\cdot\hat{e}_z, \tag{14}$$

with $h^2 = (c^2 + \frac{1}{Pr\Delta\tau})$. The right hand sides of Eqs. (13) and (14) are the $k-th$ outer residuals, $r^{\psi}_{outer}(k)$ and $r^{\xi}_{outer}(k)$ which measure the extent to which Eqs. (9) and (10) are satisfied by the $k-th$ order approximation. Given the residuals, we solve for the outer corrections, δ_k and θ_k, and then obtain a better approximation to $\psi(\tau+\Delta\tau)$ and $\xi(\tau+\Delta\tau)$. Iteration continues over the index k, until both the outer residuals and the outer corrections are small compared to ψ_k and ξ_k, that is,

$$\max(\parallel\delta_k\parallel, \parallel r^{\psi}_{outer}(k)\parallel) \leq \epsilon_{rel}(\parallel\psi(k)\parallel) + \epsilon_{abs}, \tag{15}$$

and,

$$\max(\parallel\theta_k\parallel, \parallel r^{\xi}_{outer}(k)\parallel) \leq \epsilon_{rel}(\parallel\xi(k)\parallel) + \epsilon_{abs}, \tag{16}$$

where ϵ_{rel} and ϵ_{abs} are the relative and absolute error tolerances, chosen to be 0.1 and 10^{-4} respectively in our calculations. When the convergence criteria are satisfied, ψ_{k+1} and ξ_{k+1} are set to be $\psi(\tau+\Delta\tau)$ and $\xi(\tau+\Delta\tau)$. In the numerical solution, we have found that $\Delta\tau > \Delta\tau_{max} \simeq 1.8$ will cause a numerical instability, so we have chosen $\Delta\tau < \Delta\tau_{max}$. ($\Delta\tau \ll 1.0$ during the initial transient at onset). For a given ψ_{k+1}, Eq. (14) has the exact form of Eq. (7), with $a = -c^2 - \frac{1}{Pr\Delta\tau}$, $b = 0$, $f_1 = r^{\xi}_{outer}(k)$, $f_2 = f_3 = 0$, and can be solved rapidly and accurately. Eq. (14) is almost of the form of Eq. (7) except for the non-constant term $-2g_2\psi_k - 3\psi_k^2$ in the left hand side operator. We can reduce this equation to the desired constant coefficient biharmonic form by assuming a successive approximation of the form:

$$\delta_k \simeq \delta_{k,m+1} = \delta_{k,m} + \eta_m, \tag{17}$$

where the inner correction field, $\eta_m(x,y)$, is assumed to be small compared to $\delta_{k,m}$, the $m-th$ approximation to δ_k. By substituting Eq. (17) into Eq. (13) and solving for η_m by approximating the non-constant term acting on η_m as a constant C, we obtain

$$\left[L - \frac{1}{\Delta\tau} + C\right]\eta_m = r^{\psi}_{outer}(k) - \left[L - \frac{1}{\Delta\tau} - 2g_2\psi_k - 3\psi_k^2\right]\eta_{k,m}. \tag{18}$$

The right hand side is the $m-th$ inner residual, $r^{\psi}_{inner}(k,m)$ of Eq. (18). This measures the extent to which Eq. (13) is satisfied after m iterations. The constant $C = -2g_2 < \psi_k > -3 < \psi_k^2 >$, where $<>$ denotes a spatial average over the entire system. Now Eq. (18) has the exact form of the constant coefficient biharmonic equation given in Eq.(7), with $a = 2$, $b = 1 + \frac{1}{\Delta\tau} - \epsilon - C$, $f_1 = -r^{\psi}_{inner}(k,m)$, and $f_2 = f_3 = 0$. The criterion for inner accuracy after m iterations has the following form [9] [17]:

$$\frac{\| r^{\psi}_{inner}(k,m) \|}{\| r^{\psi}_{outer}(k) \|} \leq \alpha \left[\frac{\| r^{\psi}_{outer}(k) \|}{\| r^{\psi}_{outer}(1) \|} \right]^{\beta}, \tag{19}$$

where α and β are chosen to be 0.1 and 0.5 in our numerical simulations, since the rate of convergence is not sensitive to α and β [9, 17].

We describe next the discretization of the spatial derivatives in Eqs. (9)-(10) for the geometry of interest. Since both the Laplacian and biharmonic operators have a singularity at the origin of a polar coordinate system, we have found it convenient to use a Cartesian coordinate system and approximate the boundary conditions. We have used the usual 5- and 13- point discretizations of the Laplacian and biharmonic operators on a square grid of $N \times N$ points, which is second-order accurate in the mesh spacing. We approximate the circular boundary conditions on ψ and ξ by taking $\psi(\vec{r},t) = \xi(\vec{r},t) = 0$ for $\|\vec{r}\| \geq D/2$, where $\vec{r}$ is the location of a node with respect to the center of the domain of integration, and D is the diameter of the circular domain. This approximation is presumably not dangerous since boundary effects are known to affect the bulk behavior over length scales of the order of $\epsilon^{-\frac{1}{2}}$ [13], which is large compared to the spatial discretization. Since the convective pattern has locally periodic solutions with wavelength 2π, except near the boundary, 8 or 12 grid points per wavelength are used in our numerical calculations.

Two different kinds of initial conditions are used. The first one is a gaussian distributed random initial condition with zero mean value and small variance (see below) for ψ, and ξ=0. This initial condition models the conduction state. The second type of initial conditions used is a solution from a previous run ($\psi(t_0)$, $\xi(t_0)$).

This, for example, would correspond to studying the transition from a hexagonal state to a roll state in an experiment that suddenly increased the Rayleigh number.

4 Numerical results

In this section, we report the results of our numerical calculations based on Eqs. (3)-(6) in a large aspect ratio cell, and compare the pattern evolution obtained with the experiments of Bodenschatz et al. We begin with the formation of a convecting state of hexagonal symmetry from the conducting state. Next, we present numerical evidence for the spontaneous formation of a rotating spiral pattern during the hexagon to roll transition. We also report numerical results on the formation of rotating spiral patterns during the transition from conduction to rolls.

4.1 Nucleation of a pattern with hexagonal symmetry

We consider as initial condition $\psi(\vec{r}, t = 0)$ a Gaussian random variable with zero mean and variance 10^{-6}. The forcing field chosen is $f(\vec{r}) = 0$, simply because there is no influence from the lateral boundaries before the nucleated pattern reaches the boundary. We also neglect in this case the mean flow field. We numerically solve Eq. (3) in a square domain of side $L = 128\pi$ (in our dimensionless variables, this corresponds to an aspect ratio $\Gamma = L/\pi = 128$). The differential equation is discretized on a square grid of 512×512 nodes. We use $g_2 = 0.35$ and $\Delta x = \pi/4.25$. We take $\epsilon = 0.01$ except in a small square region near the center of the cell (of size 16×16 nodes) where $\epsilon = 0.055$. This space dependent ϵ models a small localized inhomogeneity in one of the cell plates. According to the calculation by Busse [4], and our estimate of the values of the parameters in the GSH equation (see the Appendix), a hexagonal pattern should be stable for both $\epsilon = 0.01$ and $\epsilon = 0.05$. The temporal evolution of the

pattern is shown in Fig. 1. It presents an early transient behavior during which a local convective region with hexagonal symmetry has just nucleated. Six fronts of rolls, traveling away from the hexagonal patch located at the center, propagate into the conduction region. This is qualitatively similar to the experimental observations of Bodenschatz et al. [3, 18]. The observation of nucleation and growth is especially interesting since it provides an example of competition among different symmetries, i.e., a uniform conduction state as the background state, a region of hexagonal symmetry being nucleated and rolls in the front region separating the two. This situation is also interesting from the point of view of pattern selection during front propagation in dimensions higher than one. It is worth pointing out, however, that the shape of the front region obtained numerically is somewhat different than the experimental one. This difference may be attributable to the fact that the numerical value $\epsilon(\vec{r})$ used here is much larger than the experimental value. Unfortunately, it is very time consuming for us to solve the equation for the experimental value $\epsilon_{exp} \sim 10^{-4}$.

We have also estimated the speed of propagation of the front that separates the hexagonal pattern and the uniform state. This speed, at the center of the planar sides, and along their normal direction, is approximately constant in time and equals $v_{\perp} = 0.37$. The value given by marginal stability theory for the one dimensional Swift-Hohenberg equation ($g_2 = 0$) is $v_{MS} = 0.397$ [19, 20]. It will be interesting to measure the front velocity in the experiment.

4.2 Conduction to hexagon transition

In what follows, we consider a circular cell of radius $r = 32\pi$, which corresponds to an aspect ratio of $\Gamma = r/\pi = 32$. A grid with N^2 nodes has been used with spacing $\Delta x = \Delta y = 64\pi/\mathrm{N}$, and $N = 256$, with an approximate boundary conditions to mimic a circular cell as we discussed in section 3. The initial condition $\psi(\vec{r}, t = 0)$ is again a random variable, gaussianly distributed with zero mean and variance 10^{-1}. In this

case $\epsilon = 0.1$, which is also within the region in which a hexagonal pattern is stable. The forcing field $f = 0$ everywhere except at the nodes adjacent to the boundary where $f = 0.1$. This value is of the same order as a previous estimate obtained for a similar experimental setup, such that the convective heat current measured during a ramping experiment agreed with the numerical solution of the SH equation [15, 16]. Figure 2 presents the evolution of the hexagonal pattern evolution from random initial condition. Mean flow field effects have also been included in the calculation.

4.3 Hexagon to roll transition, and formation of rotating spirals

We have used the configuration shown in Fig. 2(d) as the initial condition, with exactly the same parameters and forcing field f as before ($f = 0.1$), but have increased ϵ very slowly up to $\epsilon = 0.3$: $\epsilon = 0.1 + 1.67 \times 10^{-4}t$ for $0 < t < 1200$, and $\epsilon = 0.3$ for $t > 1200$. Figure 3 shows a sequence of configurations during the early transient regime of the hexagon to roll transition. Rolls appear in the vicinity of the sidewall and tend to orient themselves parallel to it. Defects glide toward each other and invade nearby regions of hexagonal symmetry to create a region of rolls that spreads across the cell as the transition proceeds. The formation of spirals is already noticeable in Fig. 3(d).

Fig. 4 shows a continuation of the sequence of configurations shown in Fig. 3. Fig. 4(a) shows how rolls bend rapidly to form a locally disordered texture near the upper left portion of the system. Defects in the disordered texture migrate away or annihilate each other, leaving a roughly uniform patch of rolls, and eventually annihilating themselves, ending in a three-armed spiral (Figs. 4(c)-(e)). The final state of a rotating spiral (Figs. 4(e) and (f)) is remarkably similar to the one observed in the experiments, and occurs at $t \simeq 49000 \simeq 12$ horizontal diffusion times [21]. The corresponding experimental times are in the range of 10 to 20 horizontal diffusion

times.

4.4 Roll to hexagon transition

Figures 5(a)-(d) show the evolution from a initial rotating spiral to a hexagonal pattern. We have used the configuration shown in Fig. 4(f) as the initial condition, have kept the same parameters and forcing field as before ($g_2 = 0.35$, $g_m = 50.0$, $c^2 = 10.0$ and Pr=1.0), but have set $\epsilon = 0.1$. Initially, regions of hexagonal symmetry emerge near the tip and the end of the spiral, forming local domains of hexagons and then spreading across the cell. An interesting feature worth noticing during this transient period is the relative orientation between domains with different symmetries. If one uses the outer layer of hexagons in the domain to define a boundary, one can see from Fig. 5 that there is a tendency for these boundaries to be perpendicular to the direction defined by the rolls. In systems in which the evolution is governed solely by a Lyapunov functional, theoretical arguments have been given to explain analogous orientation phenomena [8]. Although these arguments do not apply in the present case, the patterns observed both in the experiments and in our numerical calculations still show that, locally, the boundary separating regions of hexagons and rolls tends to be perpendicular to the rolls. Perhaps a coupled Newell-Whitehead-Segel model (which has an associated Lyapunov functional) could be used to describe the formation of domain boundaries between hexagons and rolls [22].

4.5 Conduction to roll transition

We study in this section the formation of a set of convective roll directly from the conducting state. We use a random initial condition (gaussianly distributed with zero mean and a variance of 10^{-4}), and set ϵ=0.3. Figure 6 shows that concentric rolls are created near the sidewall and propagate inward. Small and large length scale

defects anneal out rapidly leaving a disordered structure at the center of the cell (Fig. 6(a) and (b)). Further evolution involves the annihilation of defects at the center of cell. Figures 6(c) and (d) show a two-armed rotating spiral in which all defects have been eliminated from the center of the cell. This calculation shows the importance of sidewall forcing and the geometric shape of the container for the formation of a rotating spiral.

Another interesting feature observed in the experiments that our model can also reproduce is that a stable, n-armed spiral tends toward one with fewer arms when ϵ is decreased. With the same random initial condition and parameters as in Fig. 6, we have obtained a two-armed spiral for $\epsilon = 0.3$ (Fig. 6), a one-armed spiral for $\epsilon = 0.26$ (Fig. 7), and a zero-armed spiral (concentric rolls) for $\epsilon = 0.22$.

4.6 Stability of the rotating spiral pattern

We discuss in this section the condition under which the rotating spiral is stable. Earlier work [23] established that a spiral pattern can be spontaneously formed in the absence of mean flow ($g_m = 0$), but retaining the non-Boussinesq contribution ($g_2 > 0$). The spiral pattern obtained, however, is stationary. The addition of mean flow effects is sufficient to spontaneously produce a uniformly rotating spiral. We address here the stability of an already formed rotating spiral with respect to changes in the various terms of the GSH equation.

Once the rotating spiral has been formed, we set $g_2 = 0.0$. We use the configuration shown in Fig. 7(b) as the initial condition, with exactly the same parameters ($\epsilon = 0.26$, $c^2 = 10.0$, $g_m = 50.0$, $Pr = 1.0$) and forcing field f as in Fig. 7(b). Figure 8 shows the resulting evolution of the pattern. The defect in the arms of the spiral propagates inwards as the one-armed spiral evolves to a set of concentric rolls. This result suggests that non-Boussinesq effects are needed to stabilize the spiral struc-

ture, even under the presence of mean flow. It would be very useful to replicate this observation experimentally. Further, if $f = 0$ rolls tend to align themselves normal to the sidewall, and a pattern of almost straight and parallel rolls obtains.

In summary, sidewall forcing and non-Boussinesq effects ($g_2 > 0$) are essential to produce a spiral pattern. A rotating spiral is obtained when $g_m \neq 0$. Once the rotating spiral is formed, if $g_2 = 0, g_m \neq 0$, the spiral decays to concentric rolls.

4.7 Convective current versus the number of arms in a spiral pattern

We have observed that for a given value of ϵ, the number of arms of the rotating spiral depends on the initial condition. In order to compare the convective heat current for the same value of ϵ, but for spiral patterns containing different numbers of arms, we proceed in the following way: the configurations shown in Fig. 7a (zero armed spiral for $\epsilon = 0.22$), Fig. 7b (one-armed spiral for $\epsilon = 0.26$), and Fig. 6d (two-armed spiral for $\epsilon = 0.30$) are taken as initial conditions and ϵ is set equal to $\epsilon = 0.26$. The three spiral pattern remain stable in all cases. We then calculate the convective heat current as a function of the number of arms in a spiral pattern. In Fig. 9, we compare the spatial and temporal average of the convective current $< J_{conv} >$ for the three cases discussed above. It is apparent from Fig. 9 that $< J_{conv} >$ decreases with increasing the number of arms in the spiral. Since the Nusselt number is related to the convective current by Nu=$J_{conv} + 1$, it would also be interesting to check this observation experimentally.

5 Conclusions

We have investigated a model of convection for non-Boussinesq fluids that allow patterns of various symmetries. The model used is a generalization of the Swift-Hohenberg equation that includes a quadratic term and coupling to large scale mean flows. The parameters in the equation have been chosen to match the experiments of Bodenschatz et al. on CO_2 gas [3]. An appropriate value for the control parameter ϵ takes the conduction state to an ordered hexagonal state analogous to the ones observed in experiments. We then show that upon increasing ϵ, the hexagonal state evolves into a new roll state that contains a rotating spiral pattern. The time scale to form a rotating spiral is on the time scale of 10 horizontal diffusion time. These results are also in good agreement with the experimental studies on CO_2 gas. The observation of the stationary rotating spiral pattern is not in predicated by Busse [4]. According to Busse [4], when the control parameter exceeds the bifurcation point of the hexagon-roll state, the system is expected to evolve to a stationary parallel roll state. This is because they studied the convective fluid in an infinite cell. We have given a preliminary study of the mechanism for spiral pattern formation. Our calculations illustrate the strong influence of non-Boussinesq effects, sidewall forcing, and mean flow on the appearance and stability of the rotating spiral patterns. Our results for convective current of different armed-spirals show that the final state of the rotating spiral dependents on the initial configuration. We have seen that a zero-armed, a one-armed and a two-armed rotating spiral pattern could exist for the same control parameter. This suggests the existence of multi-states for a given control parameter. Our numerical results show that the two dimensional generalized Swift-Hohenberg quation can describe quantitatively detail the three dimensional convective dynamics of a fluid beyond the Boussinesq approximation.

We conclude by suggesting some further analytical and numerical studies. It would be very useful to study how the instabilities, such as the zigzag, cross-roll, and Eckhaus instabilities are affected by the influence of the non-Boussinesq effect and the

finite size of the boundaries. It would be also very interesting to study the dynamics of the core and the tip (dislocation) of a rotating spiral, and to determine the speed of climbing motion of the tip.

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Appendix

In this appendix a detailed analysis of the various stationary solutions of the generalized Swift-Hohenberg equation is presented. In dimensionless units [11], the generalized SH model can be written as,

$$\tau_0 \frac{\partial \psi(\vec{r},t)}{\partial t} = \left[\epsilon - \frac{\xi_0^2}{4q_c^2}\left(\nabla^2 + q_c^2\right)^2\right]\psi - g_2\psi^2 - g_3\psi^3. \tag{20}$$

We set [11],

$$\psi = \sqrt{2}\sum_{j=1}^{3} Re(A_j)e^{i\theta_j}, \tag{21}$$

where $\theta_j = \vec{q}_j \cdot \vec{r}$, $\sum_{j=1}^{3}\theta_j = 0$ and A_j is a complex amplitude.

If we substitute ψ, ψ^2 and ψ^3 into Eq.(20) and keep the lowest order in the

amplitudes, we obtain

$$\tau_0\frac{\partial A_1}{\partial t} = \left[\epsilon - \xi_0^2\left(\frac{\partial}{\partial x_1} - \frac{i}{2q_c}\frac{\partial^2}{\partial y_1^2}\right)^2\right] A_1 - aA_2^*A_3^* - bA_1(|A_2|^2+|A_3|^2) - cA_1|A_1|^2, \quad (22)$$

$$\tau_0\frac{\partial A_2}{\partial t} = \left[\epsilon - \xi_0^2\left(\frac{\partial}{\partial x_2} - \frac{i}{2q_c}\frac{\partial^2}{\partial y_2^2}\right)^2\right] A_2 - aA_1^*A_3^* - bA_2(|A_1|^2+|A_3|^2) - cA_2|A_2|^2, \quad (23)$$

$$\tau_0\frac{\partial A_3}{\partial t} = \left[\epsilon - \xi_0^2\left(\frac{\partial}{\partial x_3} - \frac{i}{2q_c}\frac{\partial^2}{\partial y_3^2}\right)^2\right] A_3 - aA_1^*A_2^* - bA_3(|A_1|^2+|A_3|^2) - cA_3|A_3|^2, \quad (24)$$

where $a = \sqrt{2}g_2$, $b = 3g_3$ and $c = \frac{3}{2}g_3$ and,

$$\frac{\partial}{\partial x_j} = cos\theta_j\frac{\partial}{\partial x} + sin\theta_j\frac{\partial}{\partial y}, \quad (25)$$

$$\frac{\partial}{\partial y_j} = -sin\theta_j\frac{\partial}{\partial x} + cos\theta_j\frac{\partial}{\partial y}, \quad (26)$$

$$\theta_1 = 0, \quad \theta_2 = \frac{2\pi}{3} \quad and \quad \theta_3 = \frac{4\pi}{3}. \quad (27)$$

If we assume a uniform solution, we simply have,

$$\tau_0\frac{\partial A_1}{\partial t} = \epsilon A_1 - aA_2^*A_3^* - bA_1(|A_2|^2 + |A_3|^2) - cA_1|A_1|^2, \quad (28)$$

$$\tau_0\frac{\partial A_2}{\partial t} = \epsilon A_2 - aA_1^*A_3^* - bA_2(|A_1|^2 + |A_3|^2) - cA_2|A_2|^2, \quad (29)$$

$$\tau_0\frac{\partial A_3}{\partial t} = \epsilon A_3 - aA_1^*A_2^* - bA_3(|A_1|^2 + |A_3|^2) - cA_3|A_3|^2. \quad (30)$$

This set of equations can be written in variational form as,

$$\tau_0\frac{\partial A_i}{\partial t} = -\frac{\delta\mathcal{L}}{\delta A_i^*}. \quad (31)$$

where the Lyapunov functional $\mathcal{L}$ is given by,

$$\begin{aligned}\mathcal{L} = &-\epsilon(|A_1|^2 + |A_2|^2 + |A_3|^2)) + a(A_1^*A_2^*A_3^* + A_1A_2A_3) \\ &+b(|A_1|^2|A_2|^2 + |A_2|^2|A_3|^2 + |A_3|^2|A_1|^2) + \tfrac{c}{2}(|A_1|^4 + |A_2|^4 + |A_3|^4).\end{aligned} \quad (32)$$

The dynamical system Eqs. (28)-(30) has three stationary and homogeneous solutions:

$$Conduction\ state:$$

$$A_1 = A_2 = A_3 = 0.$$

$$Hexagonal\ state:$$

$$\begin{aligned} &A_1 = |A|e^{i\theta_1}, A_2 = |A|e^{i\theta_2}, A_3 = |A|e^{i\theta_3}, \\ &\theta_1 + \theta_2 + \theta_3 = 0, \\ &|A| = (-a - \sqrt{a^2 + 4(2b+c)\epsilon})/(2(2b+c)). \end{aligned} \tag{33}$$

$$Roll\ state:$$

$$\begin{aligned} &A_1 = |A|e^{i\theta_1}, \quad A_2 = A_3 = 0, \\ &|A| = \sqrt{\epsilon/c}. \end{aligned}$$

The linear stability of these solutions is determined by the eigenvalues of the matrix $\delta^2\mathcal{L}/\delta A_i \delta A_j$, linearized around the stationary solutions. For $\epsilon_a \leq \epsilon \leq 0$, both conduction and hexagons are stable; for $0 \leq \epsilon \leq \epsilon_r$, only hexagons are stable; for $\epsilon_r \leq \epsilon \leq \epsilon_b$ both hexagon and roll are stable; and for $\epsilon \geq \epsilon_b$, only rolls are stable. From the corresponding values of the stability boundaries obtained for the amplitude equation [24], we find,

$$\epsilon_a = -\frac{a^2}{(8b+4c)} = -\frac{2g_2^2}{15g_3}, \tag{34}$$

$$\epsilon_r = \frac{a^2 c}{(b-c)^2} = \frac{4g_2^2}{3g_3}, \tag{35}$$

$$\epsilon_b = \frac{a^2(b+2c)}{(b-c)^2} = \frac{16g_2^2}{3g_3}. \tag{36}$$

Equations (34-36) can be compared with the corresponding equation obtained by the Busse [4]. This allows to determine the coefficients a, b, c in the amplitude equation as

$$a^2 = \frac{3P^2}{R_c}, \tag{37}$$

$$b = \frac{3\Re_h - \Re_r}{2}, \tag{38}$$

$$c = \Re_r \tag{39}$$

Here $\Re_h$, $\Re_r$ and P are the constants. In the case a rigid-rigid boundary layer, we have

$$R_c = 1707, \tag{40}$$

$$\Re_h = 0.8936 + 0.04959 Pr^{-1} + 0.06787 Pr^{-2}, \tag{41}$$

$$\Re_r = 0.69942 - 0.00472 Pr^{-1} + 0.00832 Pr^{-2}. \tag{42}$$

where Pr is the Prandtl number, P is the non-Boussinesq parameter [4].

Since the system of equations (28-30) has an associated potential $\mathcal{L}$, the absolute stable state corresponds to the global minimum of $\mathcal{L}$, while metastable states correspond to local minima. The existence of the Lyapunov functional ensures that two stable phases can coexist only when they have the same value of $\mathcal{L}$. We define ϵ_T to be the value for which hexagons and the conduction state coexist, and $\epsilon_{T'}$ the value fot the coexistence of hexagons and rolls. We obtain,

$$\epsilon_T = -\frac{8}{9}\epsilon_a, \tag{43}$$

$$\epsilon_{T'} = (2b + c)|A|^2 + a|A|, \tag{44}$$

where $|A|$ is the solution of

$$3c(2b + c)|A|^3 + 2ac|A|^2 - (2b + c)|A| - a = 0. \tag{45}$$

In order to obtain the values of the coupling coefficients g_2 and g_3, we calculate the convective current J_{conv} for the various patterns. J_{conv} is given by [11],

$$J_{conv} = \sum_i |A_i|^2. \tag{46}$$

For a hexagonal pattern J_{conv} is,

$$J_{conv} = 3|A_{hex}|^2 = 3\left[\left(a + \sqrt{a^2 + 4(2b+c)\epsilon}\right)/(4b+2c)\right]^2$$
$$= 3\left[(\sqrt{2}(g_2^2/\sqrt{g_3})^{1/2} + \sqrt{2g_2^2/g_3 + 30\epsilon})/(15\sqrt{g_3})\right]^2. \tag{47}$$

For a roll pattern J_{conv} is

$$J_{conv} = |A_{roll}|^2 = \frac{\epsilon}{c} = \frac{2\epsilon}{3g_3}. \tag{48}$$

By substituting the experimental values [3] of the threshold for $\epsilon_a \approx -2.3 \times 10^{-3}$ in the previous expressions for the stability boundaries of the various patterns, we obtain, $g_2^2/g_3 \simeq 0.0345$. Furthermore, at $\epsilon = 0.02$, we have (from Fig. 2 in [3]), that $\epsilon_r \simeq 0.06$; hence $g_2^2/g_3 \simeq 0.045$. Also, $\epsilon_b \simeq 0.22$, therefore, $g_2^2/g_3 \simeq 0.0413$. We have used $g_2^2/g_3 = 0.04$ in our calculations.

By fitting the experimental convective current at $\epsilon = 0.11$ (from Fig. 1 in [3]), we obtain, $(J_{conv})_{roll} \simeq 0.16 = \frac{2\epsilon}{3g_3}$ or $g_3 \simeq 0.458$. By fitting the experimental convective current at $\epsilon = 0.02$ (from Fig. 1 in [3]) and by using $g_2^2/g_3 = 0.045$, we obtain,

$$(J_{conv})_{hex} \simeq 0.04 = 3\left[(\sqrt{2}(g_2^2/\sqrt{g_3})^{1/2} + \sqrt{2g_2^2/g_3 + 30\epsilon})/(15\sqrt{g_3})\right]^2, \tag{49}$$

or, $g_3 \simeq 0.426$.

We next discuss the calculation of the numerical parameters in the GSH equation related to large scale mean flow. The dynamical equations are,

$$\tau_0(\frac{\partial\psi}{\partial t} + \vec{U}\cdot\nabla\psi) = \left[\epsilon - \frac{\xi_0^2}{4q_c^2}\left(\nabla^2 + q_c^2\right)^2\right]\psi - g_2\psi^2 - g_3\psi^3, \tag{50}$$

and,

$$\left[\frac{\partial}{\partial t} - Pr(\nabla^2 - b^2)\right]\nabla^2\xi = g_m\left[\nabla(\nabla^2\psi)\times\nabla\psi\right]\cdot\hat{e}_z, \tag{51}$$

where mean flow velocity $\vec{U}$,

$$\vec{U} = (\partial_y\xi)\hat{e}_x - (\partial_x\xi)\hat{e}_y. \tag{52}$$

Here $\epsilon = \frac{R}{R_c} - 1$ is the reduced Rayleigh number. R_c is the critical Rayleigh number for an infinite system, and Pr is the Prandlt number. The constants τ_0 and ξ_0 are the characteristic time and length scales, q_c is the critical wave number and g_2, g_3 are the nonlinear coupling constants. b^2 is an unknown constant. Here $g_m = R_c < u_{0\perp}(z)^2 > /(q_c^2 < u_{0z}(z)\theta_0(z) >)$. We have used the fact that near onset [11],

$$[V_\perp(\vec{r}, z, t), V_z(\vec{r}, z, t), \theta(\vec{r}, z, t)] \approx \frac{1}{C} [u_{0\perp}(z)\partial_\perp, u_{0z}(z), \theta_0(z)]\, \psi(\vec{r}, t) \tag{53}$$

Here $\vec{V} = (V_\perp, V_z)$ are the velocity field and θ is the deviation of the temperature from the linear conduction profile. The functions $u_{0\perp}(z), u_{0z}(z)$ and $\theta_0(z)$ are the first eigenmodes in the vertical direction of the order parameter. Here $\vec{r}$ denotes the two-dimensional horizontal coordinate. The constant $C = \sqrt{< u_{0z}(z)\theta_0(z) > /R_c}$. The symbol $< \ >$ means here an average over the vertical direction. now rescale $\vec{r}' = q_c\vec{r}$, $t' = \frac{q_c^2\xi_0^2}{4\tau_0}t$, $\psi' = \frac{2\sqrt{g_3}}{q_c\xi_0}\psi$, $\epsilon' = \frac{4}{q_c^2\xi_0^2}\epsilon$, $\xi' = \frac{g_3}{g_m\tau_0 q_c^2}\xi$. The rescaled GSH equation with large scale flow field becomes,

$$\frac{\partial\psi'}{\partial t'} + g_m'\vec{U}' \cdot \nabla\psi' = \left[\epsilon' - \left(\nabla'^{\,2} + 1\right)^2\right]\psi' - g_2'\psi'^{\,2} - \psi'^{\,3}, \tag{54}$$

$$\left[\frac{\partial}{\partial t'} - Pr'(\nabla'^{\,2} - c'^{\,2})\right]\nabla'^{\,2}\xi' = \left[\nabla'(\nabla'^{\,2}\psi') \times \nabla'\psi'\right] \cdot \hat{e}_z, \tag{55}$$

where $g_2' = (2g_2)/(\xi_0 q_c\sqrt{g_3})$, $g_m' = (4\tau_0^2 g_m q_c^2)/(g_3\xi_0^2)$, $Pr' = (4\tau_0/\xi_0^2)Pr$, and $c'^{\,2} = b^2/q_c^2$. From the experiments on CO_2 [3], we use $R_c = 1707, q_c = 3.117, \xi_0^2 = 0.148, Pr = 1, \tau_0 = 0.07693 (\tau_0 = \frac{Pr+0.5117}{19.65 Pr}$ for rigid-rigid boundary conditions), $g_m = 2.52$ (for rigid-rigid boundary conditions), $g_2^2/g_3 = 0.04$, and $g_3 = 0.458$. We finally have $g_2' = 0.335$, $Pr' = 2.079$, $g_m' = 8.548$, $\epsilon' = 2.7818\epsilon$, and $c'^{\,2}$ is an unknown constant.

To recapitulate, we use in our numerical solution $g_2' = 0.35$, $g_m' = 50$, $c'^{\,2} = 10$

and $Pr' = 1.0$. For these values the stability boundaries of the various patterns are,

$$
\begin{aligned}
&\epsilon'_a = -0.008167, \text{ or, } \epsilon_a = -0.00293, \\
&\epsilon'_r = 0.1633, \text{ or, } \epsilon_r = 0.0587, \\
&\epsilon'_b = 0.6533, \text{ or, } \epsilon_b = 0.2348, \\
&\epsilon'_T = -0.00726, \text{ or, } \epsilon_T = -0.00261, \\
&\epsilon'_{T'} = 0.24, \text{ or, } \epsilon_{T'} = 0.0863.
\end{aligned}
\tag{56}
$$

Note that we have omitted the primes in the Equations (3-6).

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Figure captions

Figure 1. Nucleation of a pattern of hexagonal symmetry in a square cell of aspect ratio $\Gamma = 128$. The values of the parameters used are $g_2 = 0.35, \epsilon = 0.01$ and $f = 0$. In a small square region at the center of the cell, $\epsilon = 0.055$. The time shown is $t = 611$ and dark (white) areas represent regions in which ψ is positive (negative).

Figure 2. Hexagonal pattern obtained from a random initial condition in a cylindrical cell of aspect ratio $\Gamma = 64$. The values of the parameters used are $g_2 = 0.35$, $g_m = 50$ and $\epsilon = 0.1$. A forcing field localized at the boundary $f = 0.1$ has been used. Four different times, (a), $t = 1.3$; (b), $t = 51.2$; (c), $t = 1049.7$; and, (d), $t = 4649.7$ are shown.

Figure 3. This figure shows the early stages of hexagon to roll transition produced by suddenly changing ϵ from $\epsilon = 0.1$ to $\epsilon = 0.3$, in a cylindrical cell of aspect ratio $\Gamma = 64$. The initial condition is the uniform hexagonal pattern shown in Fig. 2a. Four different times, (a), $t = 480$; (b), $t = 720$; (c), $t = 840$; and, (d), $t = 960$ are shown. Rolls appear near defects and sidewall boundaries and spread through the cell as the transition proceeds.

Figure 4. Formation of a rotating three-armed spiral in a cylindrical cell of aspect ratio $\Gamma = 64$, with $g_2 = 0.35$, $g_m = 50$, $\epsilon = 0.3$ and $f = 0.1$. The configurations shown are continuation of those in Fig. 3. The times shown are (a), t=1400; (b), t= 7440; (c), t=18000; (d), t=41040; (e), t=48240; and, (f), t=64080. The final rotating spiral pattern is shown in (e) and (f) is stable.

Figure 5. Formation of a hexagonal pattern from a three-armed rotating spiral (Fig. 4(f)), with $g_2 = 0.35$, $g_m = 50$, $\epsilon = 0.1$ and f=0.1. An interesting feature to note is that the orientation of the hexagonal domains tends to be normal to the rolls. Four configurations during th early transition period are shown here: (a), t=649; (b), t=1299; (c), t=2130; and, (d), t=3090.

Figure 6. Formation of a two-armed rotating spiral from random initial conditions, with $g_2 = 0.35$, $g_m = 50$, $\epsilon = 0.3$ and $f = 0.1$. The configurations are shown at (a), t=70.1; (b), t=190.7; (c), t=310.7; and, (d), t=1990.7.

Figure 7. Formation of a zero-armed, and a one-armed rotating spiral pattern obtained from a random initial condition with different values of ϵ from Fig. 6. All the other parameters are the same as in Fig. 6. (a), a zero-armed spiral with $\epsilon = 0.22$, and (b), a one-armed spiral with $\epsilon = 0.26$.

Figure 8. Study of the stability of the spiral pattern. We use the one-armed spiral shown in Fig. (7b) as initial condition, switch g_2 from g_2=0.35 to g_2=0.0 and keep all the other parameters unchanged. Concentric rolls propagate inwards as the core of the one-armed spiral starts shrinking. Finally the one-armed spiral decays to a set of concentric rolls. The times shown are (a), t=0; (b), t= 180; (c), t= 252; and, (d), t= 288.

Figure 9. Convective heat current J_{conv} versus the number of arms for the same value of $\epsilon = 0.26$ The average convective current decreases with increasing the number of arms in the spiral.